C:\stnweb\Queries\456.str

```
17 19 20
                21
                     52
                         53
                             54
                                 57
ring nodes :
    1 2
          3 4
                5
                    6
                       7
                         8
                             9
                                11
                                    12
                                        13
                                             14
                                                 15
                                                     16
                                                         22
                                                             23
                                                                  24
                                                                      25
                                                                          26
                                                                              28
    29
                   34 35
       30
           31
                32
                            36 37 38 40 41 42 43 45 46 47 48
                                                                           49
    58
chain bonds :
    3-57
          8-12
                15-17
                        19-20
                               20-21
                                     52-53
                                              53-54
ring bonds :
    1-2 1-6 2-3
                  3 - 4
                         4-5
                             5-6
                                   5-7
                                        6-9 7-8 8-9
                                                       11-12
                                                              11-16
                                                                     12-13
    13-14
           14-15
                  15-16
                          22-23
                                 22-26
                                        23-24
                                                24-25
                                                       25-26
                                                              28-29
                                                                      28 - 32
    29-30
           30-31
                  31-32
                          34 - 35
                                 34 - 38
                                        35-36
                                                36-37
                                                       37-38
                                                              40-41
    41-58
           42-43
                  42-58
                          45-46
                                 45-49
                                        46-47
                                                47 - 48
                                                       48-49
exact/norm bonds :
    1-2 1-6 2-3
                  3 - 4
                         3-57 4-5 5-6
                                        5-7
                                               6-9 7-8 8-9
                                                              8-12
                                                                     15-17
                  22-23
    19-20 20-21
                          22-26
                                 23-24
                                        24-25
                                               25-26
                                                       28-29
                                                              28-32
                                                                      29-30
    30-31
           31 - 32
                  34 - 35
                          34 - 38
                                 35-36
                                        36-37
                                               37-38
                                                       40-41
                                                              40-43
                                                                      41-58
    42-43
           42-58
                 45-46
                          45-49
                                 46-47
                                        47-48
                                               48-49
                                                       52-53
                                                              53 - 54
normalized bonds :
    11-12
          11-16
                 12-13
                          13-14
                                 14-15
                                        15-16
isolated ring systems :
    containing 1 : 11 :
```

G1:CH, N

chain nodes :

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 40:Atom 41:Atom 42:Atom 43:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 52:CLASS 53:CLASS 54:CLASS 57:CLASS 58:Atom

```
C:\stnweb\Queries\7.str
```

```
chain nodes :
   17 19 20
             21 23
                     24
                         25
ring nodes :
   1 2 3 4
              5 6 7 8 9 11 12 13 14 15 16
chain bonds :
   3-28 8-12 15-17 19-20 20-21 23-24 24-25
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13
   13-14 14-15 15-16
exact/norm bonds :
   1-2 1-6 2-3 3-4 3-28 4-5 5-6 5-7 6-9 7-8 8-9 8-12 15-17
   19-20 20-21 23-24 24-25
normalized bonds :
   11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
   containing 1 : 11 :
G1:CH, N
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

19:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

20:CLASS 21:CLASS 23:CLASS 24:CLASS 25:CLASS 28:CLASS

G2:Hy, [*1], [*2]

Match level :

	•			
. • .		•		
	(*)			

* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * *						
NEWS	1			Web Page URLs for STN Seminar Schedule - N. America						
NEWS	2			"Ask CAS" for self-help around the clock						
NEWS	3	JAN	27	Source of Registration (SR) information in REGISTRY updated						
				and searchable						
NEWS	4	JAN	27	A new search aid, the Company Name Thesaurus, available in						
				CA/CAplus						
NEWS	5	FEB	05	German (DE) application and patent publication number format						
				changes						
NEWS	6	MAR	03	MEDLINE and LMEDLINE reloaded						
NEWS	7	MAR	03	MEDLINE file segment of TOXCENTER reloaded						
NEWS	8	MAR	03	FRANCEPAT now available on STN						
NEWS	9	MAR		Pharmaceutical Substances (PS) now available on STN						
NEWS	10	MAR	29	WPIFV now available on STN						
NEWS	***************************************		29	New monthly current-awareness alert (SDI) frequency in RAPRA						
NEWS				PROMT: New display field available						
NEWS	13	APR	26	IFIPAT/IFIUDB/IFICDB: New super search and display field						
				available						
	1-60-	APR		LITALERT now available on STN						
NEWS	15	APR	27	NLDB: New search and display fields available						
NEWS	16			PROUSDDR now available on STN						
NEWS	17	May	19	PROUSDDR: One FREE connect hour, per account, in both May						
				and June 2004						
NEWS		-		EXTEND option available in structure searching						
NEWS		-		Polymer links for the POLYLINK command completed in REGISTRY						
NEWS	20	May	17	FRFULL now available on STN						
NEWS	EXP	RESS	MAR	CH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT						
			MAC	CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),						
			AND	CURRENT DISCOVER FILE IS DATED 26 APRIL 2004						
NEWS	HOU	RS	STN	Operating Hours Plus Help Desk Availability						
NEWS	INT	ER	Gen	neral Internet Information						
NEWS	LOG:	IN		lcome Banner and News Items						
NEWS		1E		ect Dial and Telecommunication Network Access to STN						
NEWS	WWW		CAS	World Wide Web Site (general information)						
Enter	NEW	s fol	lowe	ed by the item number or name to see news on that						
speci				a by the reem number of name to see news on that						
-Peci	(-opic	•							

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FILE 'HOME' ENTERED AT 12:29:10 ON 17 MAY 2004

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:29:18 ON 17 MAY 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1 DICTIONARY FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

=> s 11

SAMPLE SEARCH INITIATED 12:37:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 587 TO ITERATE

100.0% PROCESSED 587 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

STR

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 10

10287 TO 13193

PROJECTED ANSWERS:

899 TO 1901

L2 50 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 12:37:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11981 TO ITERATE

100.0% PROCESSED 11981 ITERATIONS SEARCH TIME: 00.00.01

1375 SEA SSS FUL L1

1375 ANSWERS

=> file hcaplus

L3

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 160.46 160.67

FULL ESTIMATED COST

160.46 160.67

FILE 'HCAPLUS' ENTERED AT 12:37:16 ON 17 MAY 2004
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FILE COVERS 1907 - 17 May 2004 VOL 140 ISS 21 FILE LAST UPDATED: 16 May 2004 (20040516/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 776 L3

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.36 163.03

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:37:21 ON 17 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1 DICTIONARY FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter Http://www.cas.org/ONLINE/DBSS/registryss.html

=> L5 STRUCTURE UPLOADED

=> 15
L5 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d 15

L5 HAS NO ANSWERS

=> s 15

SEARCH FAILED DUE TO A STRUCTURE QUERY ERROR
The structure query could not be searched. Please review and revise
your structure query, especially checking the variable definitions and
attachments. In rare instances the failure may be due to a system
problem. Please contact your local STN Help Desk if you need
assistance.

=> L6

STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6

=> s 16

SEARCH FAILED DUE TO A STRUCTURE QUERY ERROR

The structure query could not be searched. Please review and revise your structure query, especially checking the variable definitions and attachments. In rare instances the failure may be due to a system problem. Please contact your local STN Help Desk if you need assistance.

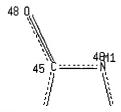
=> L7

STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

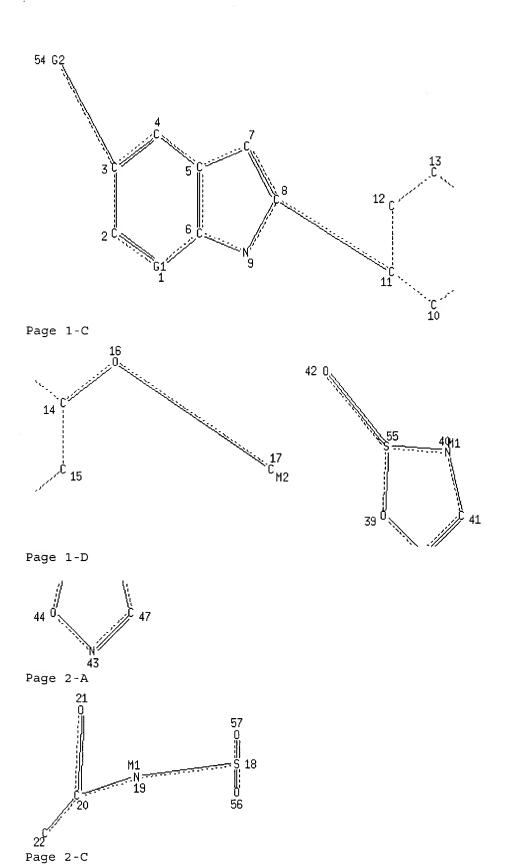
L7 STR



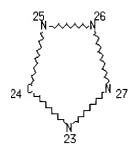
Page 1-A

60 C M1 N 61

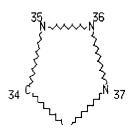
Page 1-B

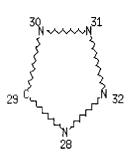


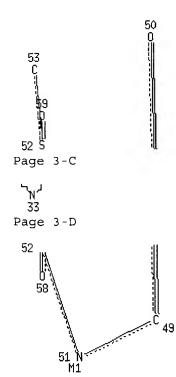




Page 2-D

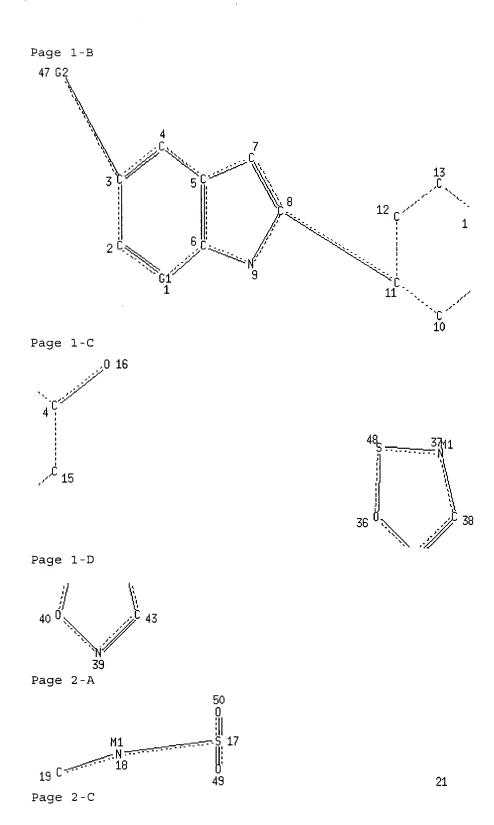




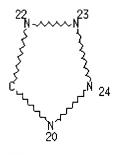


Page 4-0				
VAR G1=6				
VAR G2=1	.8/2	24/28/36	5/41/	47/49
NODE ATT	RIE	BUTES:		
HCOUNT	IS	M2	AT	17
HCOUNT	IS	Ml	AT	19
HCOUNT	IS	M1	AT	40
HCOUNT	IS	M1	AT	46
HCOUNT	IS	M1	AT	51
HCOUNT	IS	Ml	AT	60
NSPEC	IS	R	ΑT	1
NSPEC	IS	R	AΤ	2
NSPEC	IS		AΤ	3
NSPEC	IS		AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
	IS			
NSPEC		R	TA	9
NSPEC	IS	R	TA	10
NSPEC	IS	R	AT	11
NSPEC	IS		$\mathbf{T}\mathbf{A}$	12
NSPEC	IS		AT	13
NSPEC	IS		ΑT	14
NSPEC	IS	R	AT	15
NSPEC	IS	C	AT	16
NSPEC	IS	C	\mathtt{AT}	17
NSPEC	IS	C	AT	18
NSPEC	IS	C	AT	19
NSPEC	IS	C	AΤ	20
NSPEC	IS	C	AT	21
NSPEC	IS	RC	AT	22
NSPEC	IS	R	AT	23
NSPEC	IS	R	ΑT	24
NSPEC	IS	R	AΤ	25
NSPEC	IS	R	AΤ	26
NSPEC	IS	R	AT	27
NSPEC	IS	R	AT	28
NSPEC	IS	R	AT	29
NSPEC	IS	R	AT	30
NSPEC	IS	R	AT	31
NSPEC	IS			32
		R	AT	33
NSPEC	IS	R	AT	
NSPEC	IS	R	AT	34
NSPEC	IS	R	AT	35
NSPEC	IS	R	AT	36
NSPEC	IS	R	TA	37
NSPEC	IS	R	AT	38
NSPEC	IS	R	AT	39
NSPEC	IS	R	AT	40
NSPEC	IS	R	AT	41
NSPEC	IS	C	AT	42
NSPEC	IS	R	AT	43
NSPEC	IS	R	AT	44
NSPEC	IS	R	AT	45
NSPEC	IS	R	AT	46
NSPEC	IS	R	AΤ	47
NSPEC	IS	C	AT	48
NSPEC	IS	C	AT	49
NSPEC	IS	C	AT	50
		-		

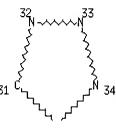
```
NSPEC IS C
                AT 51
NSPEC IS C
                 AT 52
NSPEC IS RC AT 53
NSPEC IS C AT 54
NSPEC IS R
                AT 55
NSPEC IS C
                AT 56
NSPEC IS C
                 AT 57
NSPEC IS C
                 AT 58
      IS C AT 59
NSPEC
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 16 17 18 19 20 21 22 42 48 49 50 51 52 53 56 57 58
         59
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 1 11
NUMBER OF NODES IS 61
STEREO ATTRIBUTES: NONE
=> s 17
SAMPLE SEARCH INITIATED 12:59:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE
100.0% PROCESSED
                      7 ITERATIONS
                                                             0 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                       BATCH **COMPLETE**
PROJECTED ITERATIONS:
                               7 TO 298
PROJECTED ANSWERS:
                               O TO
             0 SEA SSS SAM L7
L8
=> s 17 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:s 17 full
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
FULL SEARCH INITIATED 13:00:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -
                              223 TO ITERATE
100.0% PROCESSED
                    223 ITERATIONS
                                                             0 ANSWERS
SEARCH TIME: 00.00.01
L9
             0 SEA SSS FUL L7
=>
L10
       STRUCTURE UPLOADED
=> d 110
L10 HAS NO ANSWERS
L10
               STR
Page 1-A
 53 C M1 N 54
```

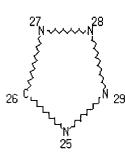


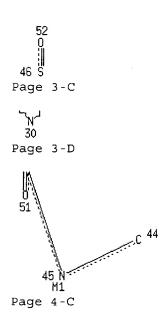




Page 2-D







VAR G1=5	3/5	4		
VAR G2=1			3/38/	43/44
NODE ATT				,
HCOUNT	IS	M1	AΤ	18
HCOUNT	IS	M1	AT	37
HCOUNT	IS	M1	ΑT	42
HCOUNT	IS	M1	ΑT	45
HCOUNT	IS	M1	AT	53
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12
NSPEC	IS	R	AT	13
NSPEC		R	AT	14
NSPEC	IS	R	AT	15
NSPEC	IS	C	AT	16
NSPEC	IS	C	AT	17
NSPEC	IS	C	AT	18
NSPEC	IS	C	AT	19
NSPEC	IS	R	AT	20
NSPEC	IS	R R	AT	21
NSPEC	IS			22
NSPEC	IS	R	AT	23
NSPEC		R	AT	24
		R	AT	25
NSPEC NSPEC		R	AT	25 26
NSPEC	IS	R	AT	27
NSPEC		R	AT	
	IS IS	R	AT	28
NSPEC NSPEC		R R	AT	29 30
NSPEC	IS IS	R R	AT AT	31
				32
NSPEC	IS	R	AT	
NSPEC NSPEC	IS	R	AT	33
NSPEC	IS IS	R	AT AT	34 35
NSPEC		R	AT	36
NSPEC	IS	R	AT	37
NSPEC		R		38
NSPEC		R R	AT	39
NSPEC		R R	AT	40
NSPEC NSPEC			AT	41
NSPEC		R	AT	42
		R	AT	
NSPEC NSPEC		R	AT	43 44
	IS	C	AT	
NSPEC	IS	C	AT	45
NSPEC	IS	C	AT	46
NSPEC	IS	C	AT	47
NSPEC		R	AΤ	48
NSPEC		C	AT	49
NSPEC		C	AT	50
NSPEC		C	TA	51
NSPEC	IS	С	AT	52

DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 16 17 18 19 44 45 46 49 50 51 52
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 11

NUMBER OF NODES IS 54

STEREO ATTRIBUTES: NONE

=> s 110

SAMPLE SEARCH INITIATED 13:01:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 119 TO 641
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s 110 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:01:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 563 TO ITERATE

100.0% PROCESSED 563 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=>

L13 STRUCTURE UPLOADED

=> d 113

L13 HAS NO ANSWERS

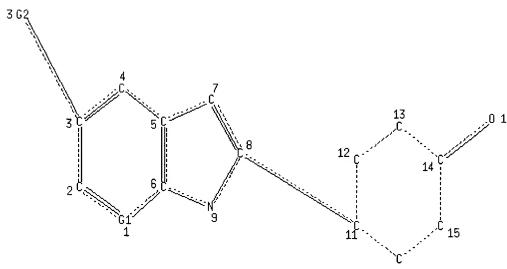
L13 ST

Hy 30

28 C M1 N 29

Page 1-A

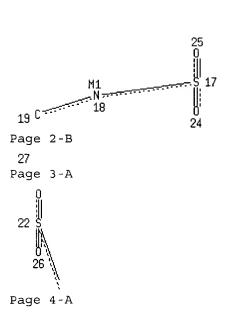
2



Page 1-B

6 Page 1-C

C 10



```
21 N 20
Page 4-B
VAR G1=28/29
VAR G2=30/17/20
NODE ATTRIBUTES:
HCOUNT
      IS M1
                 AT
                      18
HCOUNT IS M1
                 AT
                      21
HCOUNT IS M1
                  AT
                      28
                 AΤ
NSPEC
       IS R
                 AT
                       2
NSPEC
       IS R
NSPEC
      IS R
                 AT
NSPEC
       IS R
                 AT
       IS R
NSPEC
                 AT
       IS R
                 AT
NSPEC
                       6
NSPEC
       IS R
                 AT
                       7
                 ΑT
                       8
NSPEC
       IS R
                       9
NSPEC
       IS R
                 AT
NSPEC
       IS R
                 AT
                      10
NSPEC
       IS R
                 AT
                      11
                 AT
NSPEC
       IS R
                      12
NSPEC
       IS R
                  AT
                      13
                  AT
NSPEC
       IS R
                      15
NSPEC
       IS R
                  AT
NSPEC
       IS C
                  AT
                      16
NSPEC
       IS C
                 AT
                      17
NSPEC
       IS C
                 AT
                      18
NSPEC
        IS C
                 AT
                      19
NSPEC
        IS C
                 AT
                      20
NSPEC
       IS C
                 AT
                      21
NSPEC
       IS C
                 AT
                      22
NSPEC
       IS C
                 AT
                      23
NSPEC
       IS C
                  AT
                      24
        IS C
                  AT
                      25
NSPEC
NSPEC
        IS C
                  AT
                      26
                  AT
NSPEC
        IS C
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 16 17 18 19 20 21 22 24 25 26 27 30
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
=> s 113
SAMPLE SEARCH INITIATED 13:04:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1817 TO ITERATE
                                                               0 ANSWERS
                    1000 ITERATIONS
 55.0% PROCESSED
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
```

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

33784 TO 38896

PROJECTED ANSWERS:

0 TO

L14

0 SEA SSS SAM L13

=> s 113 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: γ FULL SEARCH INITIATED 13:04:16 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 35679 TO ITERATE

100.0% PROCESSED 35679 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.02

1.15

6 SEA SSS FUL L13

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

483.90 646.93

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FILE COVERS 1907 - 17 May 2004 VOL 140 ISS 21 FILE LAST UPDATED: 16 May 2004 (20040516/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 115

L16 6 L15

=> s 116 and priestley, e?/au

64 PRIESTLEY, E?/AU

L17 0 L16 AND PRIESTLEY, E?/AU

=> s 115 and decicco, c?/au

6 L15

126 DECICCO, C?/AU

L18

0 L15 AND DECICCO, C?/AU

=> s 115 and hudyma, t?/au

6 L15

45 HUDYMA, T?/AU L19 0 L15 AND HUDYMA, T?/AU

=> d l15, ibib abs fhitstr, 1-6 YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:end

=> file hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 7.08 654.01

FULL ESTIMATED COST

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FILE COVERS 1907 - 17 May 2004 VOL 140 ISS 21 (20040516/ED) FILE LAST UPDATED: 16 May 2004

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

L4

(FILE 'HOME' ENTERED AT 12:29:10 ON 17 MAY 2004)

FILE 'REGISTRY' ENTERED AT 12:29:18 ON 17 MAY 2004

STRUCTURE UPLOADED L1

50 S L1 L2

1375 S L1 FULL 1.3

> FILE 'HCAPLUS' ENTERED AT 12:37:16 ON 17 MAY 2004 776 S L3

FILE 'REGISTRY' ENTERED AT 12:37:21 ON 17 MAY 2004

STRUCTURE UPLOADED L5

L6 STRUCTURE UPLOADED

L7STRUCTURE UPLOADED

L8 0 S L7

0 S L7 FULL 1.9

STRUCTURE UPLOADED L10

0 S L10 L11

0 S L10 FULL L12

STRUCTURE UPLOADED L13

0 S L13 L14

6 S L13 FULL T₁15

FILE 'HCAPLUS' ENTERED AT 13:04:21 ON 17 MAY 2004

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L16 6 S L15

L17 0 S L16 AND PRIESTLEY, E?/AU

L18 0 S L15 AND DECICCO, C?/AU

L19 0 S L15 AND HUDYMA, T?/AU
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FILE 'HCAPLUS' ENTERED AT 13:05:52 ON 17 MAY 2004

=> d l16, ibib abs fhitstr, 1-6

L16 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1997:238314 HCAPLUS

DOCUMENT NUMBER: 126:225300

DOCUMENT NUMBER: 126:225300

TITLE: Preparation of benzazoles as radioprotectors.

INVENTOR(S): Martin, Roger Francis; Kelly, David Patterson; White,

Johnathon Michael

PATENT ASSIGNEE(S): Peter Maccallum Cancer Institute, Australia

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

								APPLICATION NO. DATE									
WO	9704	776		A1 19970213				WO 1996-AU467				19960726					
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														KR,			
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		SD,			•		•										
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OTHER SOURCE(S): MARPAT 126:225300

GI

AB Use of title compds. [I; X = (substituted) aminoalkyl, alkylene, interactive group; Y, Z = N, O, S CR; R = H, (substituted) alkyl, alkenyl;

dotted line = double bond unless the attached Y or Z group = O or S in which case it is a single bond; d R1-R11 = H, a sterically hindering group and an electron donating group; any 2 of R1 R11, Y, Z, NH and R may form a (substituted) ring which may contain heteroatoms, provided that ≥ 1 of R1-R11 = electron donating group and that when X = NMe, Y and Z = N and R1, R2, and R4-R11 = H, then R3 \neq OH or OCH2Me] as radioprotectants, is claimed. Thus, 2-amino-4-(1-piperidinyl)amine and 4-dimethylamino-1-[5-(iminoethoxy) methylbenzimidazol-2-yl]benzene hydrochloride (prepn. given) were refluxed 3 h in HOAc/EtOH to give 4-dimethylamino-1-[5-[5-(piperidin-1-yl)benzimidazol-2-yl]benzimidazol-2-yl]benzene. The latter at 17 μM in cell culture studies gave a protection factor of 2.7-2.8.

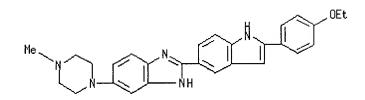
IT 188247-18-9P

RN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

188247-18-9 HCAPLUS

1H-Benzimidazole, 2-[2-(4-ethoxyphenyl)-1H-indol-5-yl]-5-(4-methyl-1-CNpiperazinyl) - (9CI) (CA INDEX NAME)



ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

(prepn. of benzazoles as radioprotectors)

Full Citana References

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

1995:647297 HCAPLUS

123:143666

Synthesis of 5- and 6-membered heterocycles by a

strategy combining SNAr and SRN1 reactions

Beugelmans, Rene; Chbani, Mohamed AUTHOR(S):

Institut Chimie Substances Naturelles, CNRS, CORPORATE SOURCE:

Gif-sur-Yvette, 91198, Fr.

SOURCE:

Bulletin de la Societe Chimique de France (1995),

132(3), 306-13

CODEN: BSCFAS; ISSN: 0037-8968

PUBLISHER: Elsevier Journal DOCUMENT TYPE: French LANGUAGE:

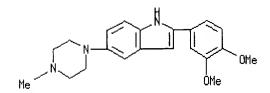
The SRN1 mechanism is compatible with many substituents on the benzenic substrate and allows SRN1 reactions to be combined with SNAr reactions in a strategy which brings together their corresponding synthetic advantages. Thus, compds. contg. benzene fused to 5- or 6-membered heterocycles contg. N (indoles), N and P (benzazaphospholes) and N and S (benzothiazines) are readily obtained.

IT 166818-63-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 5- and 6-membered heterocycles by a strategy combining SNAr and SRN1 reactions)

RN166818-63-9 HCAPLUS

CN 1H-Indole, 2-(3,4-dimethoxyphenyl)-5-(4-methyl-1-piperazinyl)- (9CI) INDEX NAME)



L16 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1

1991:679809 HCAPLUS

DOCUMENT NUMBER:

115:279809

TITLE:

Preparation of 2-phenylindole derivatives as

lipoxygenase inhibitors

INVENTOR (S):

Suzuki, Yasushi; Hasegawa, Yukio; Sato, Michitaka; Yamamoto, Norio; Hasumi, Koichi; Shidara, Kazuhiro;

Miyasaka, Katsuhiko; Kenjo, Takashi; Miyazawa,

Katsuhiko; Et, Al.

PATENT ASSIGNEE(S):

Teikoku Hormone Mfg. Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 03188064	A2	19910816	JP 1989-326634	19891216		
JP 2894617	B2	19990524				
PRIORITY APPLN. INFO.	:		JP 1989-326634	19891216		

OTHER SOURCE(S):

MARPAT 115:279809

GI

$$R^2$$
 R^3
 R^4
 R^5
 $CMe 3$
 $Et0 C$
 $CMe 3$
 OH
 OH
 Me
 II

2-Phenylindole derivs. [I; R1 = H, alkyl; R2-R4 = H, halo, alkyl, alkoxy, etc.; R5 = H, alkyl], effective lipoxygenase and cyclooxygenase inhibitors, are prepd. Refluxing a mixt. of 60 g ketone II and 55 g 4-AcNHC6H4NHNH2.HCl in Me2CHOH gave 78 g I (R1 = Me, R2 = R3 = R5 = H, R4 = 5-AcNH), which showed 82% inhibition of 5-HETE at 10 μM. Also prepd. and tested were 25 addnl. I.

IT 137614-73-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as lipoxygenase inhibitor)

RN 137614-73-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[2-[3-(1,1-dimethylethyl)-4-hydroxy-5-methylphenyl]-3-methyl-1H-indol-5-yl]- (9CI) (CA INDEX NAME)

L16 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER:

113:171973

1990:571973 HCAPLUS

DOCUMENT NUMBER: TITLE:

Nonsteroidal cardiotonics. 3. New

4,5-dihydro-6-(1H-indol-5-yl)pyridazin-3(2H)-ones and related compounds with positive inotropic activities

AUTHOR (S):

Mertens, Alfred; Friebe, Walter Gunar;

Mueller-Beckmann, Bernd; Kampe, Wolfgang; Kling,

Lothar; Von der Saal, Wolfgang

CORPORATE SOURCE:

Dep. Chem., Boehringer Mannheim G.m.b.H., Mannheim,

6800, Germany

SOURCE:

Journal of Medicinal Chemistry (1990), 33(10), 2870-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE:

LANGUAGE:

Journal English

OTHER SOURCE(S):

CASREACT 113:171973

GΙ

A series of substituted indolyldihydropyridazinones I (R = Ph, CO2Et, 3-, AB 4-pyridyl, 4-MeC6H4; R1 = H, Me, Et, CHMe2; R2 = H, Me) and related compds. were synthesized and evaluated for pos. inotropic activity. In rats, most of these indole derivs. produced a dose-related increase in myocardial contractility with little effect on heart rate and blood pressure. I (R = 4-pyridyl, R1 = H; R2 = Me), (II, BM 50.0430), was further investigated in cats. The increase in contractility in this animal model was not mediated via stimulation of β -adrenergic receptors. After oral administration of 1 mg/kg to conscious dogs, II and pimobendan were still active after 6.5 h. However, the cardiotonic effect of II was at least 2-fold that of pimobendan after this period of time. The structural requirements for optimal cardiotonic activity within this class of indole derivs. are a heterocyclic arom. ring in position 2, a hydrogen or a Me group in position 3 and a dihydropyridazinone ring system in position 5 of the indole.

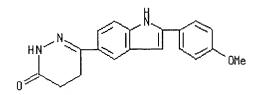
IT 129593-70-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and inotropic activity of)

RN 129593-70-0 HCAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-6-[2-(4-methoxyphenyl)-1H-indol-5-yl]-(9CI) (CA INDEX NAME)



HCAPLUS COPYRIGHT 2004 ACS on STN ANSWER 5 OF 6

Text ACCESSION NUMBER:

1984:209577 HCAPLUS

DOCUMENT NUMBER:

100:209577

TITLE:

Syntheses of antimicrobial biscationic 2-(phenoxyphenyl)indoles and -1-benzofurans

AUTHOR (S):

Dann, Otto; Ruff, Juergen; Wolff, Hans Peter;

Griessmeier, Helmut

CORPORATE SOURCE:

Inst. Pharm. Lebensmittelchem., Univ.

Erlangen-Nurnberg, Erlangen, D-8520, Fed. Rep. Ger.

Liebigs Annalen der Chemie (1984), (3), 409-25

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

German

OTHER SOURCE(S):

CASREACT 100:209577

GI

Ten 2-(phenoxyphenyl)indoles and 4 2-(phenoxyphenyl)-1-benzofurans with AΒ terminal amidinium or imidazolinium groups, e.g. I and II, were prepd. as antimicrobials. Thus, 4,2-Br(O2N)C6H3CH2COC6H4(OC6H4Br-p)-p, prepd. from 4,3-Br(O2N)C6H3CH2CO2H and p-BrC6H4OPh, underwent reductive cyclization followed by reaction with CuCN to give the indole III which was aminated with NH3 to give I.

IT 90178-91-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

90<u>178</u>-9<u>1</u>-9 HCAPLUS RN

1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-CN imidazol-2-yl)phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

2 HCl

L16 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

1983:569063 HCAPLUS

99:169063

Inhibitory activity of diarylamidine derivatives on

murine leukemia L1210 cell growth

AUTHOR(S): Balzarini, Jan; De Clercq, Erik; Dann, Otto

CORPORATE SOURCE: Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain,

B-3000, Belg.

SOURCE: Investigational New Drugs (1983), 1(2), 103-15

CODEN: INNDDK; ISSN: 0167-6997

DOCUMENT TYPE:

LANGUAGE:

Journal English

GI

A series of 96 diarylamidine and diarylamidazoline derivs., mostly I (X =AB NH, O, S, SO2, CH2; Y = CH, CNH2, N, etc.; R1 and R2 = amidino, imidazolino, etc.; Z = CH:CH, PhO, CONH, NH, etc; n = 0 or 1), II (R1 and R2 = amidino or imidazolino; Z = CH:CH, NHN:N, etc.), III (X = O, S, or NH; Y = CH, CMe, N; R1 and R2 = amidino or imidazolino), and IV (X = NH; Y)= CH; Z = CH:CH; R1 and R2 = imidazolino; n = 0 or 1), were tested for antitumor activity against murine leukemia L1210 cells. Structure-function anal. revealed that the antitumor activity of the diarylamidines depended on the planarity of the mol., the presence of amidino or, preferably, imidazolino groups or both aryl moieties, the nature of the bridge connecting the 2 aryl moieties, and the nature of the aryl moieties (preferably benzofuren or benzo[b]thiophene. Thus, (6-(2-imidazolin-2-yl)-2-[4-(2-imidazolin-2-yl)phenyl]benzo[b]thiophene (I; X = S; Y = CH; R1 = R2 = imidazolino; n = 0) [73819-21-3] was the most potent inhibitor of L1210 cell growth. The inhibitory effects of diarylamidines on L1210 cell proliferation may at least partly involve an

inhibition of DNA synthesis. 2,2'-Vinylenedi-1-benzofuran-5-carboxamidine (III; X = O; Y = CH; Z = CH:CH; R1 = R2 = amidino) [65426-90-6] exhibited potent antitumor activity in vitro and in vivo in L1210-inoculated mice.

IT 87559-26-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(neoplasm inhibitory activity of, structure in relation to)

RN <u>87559-26-0</u> HCAPLUS

CN 1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-imidazol-2-yl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

=> file caol SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 35.62 689.63 FULL ESTIMATED COST TOTAL SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SESSION ENTRY -4.16 CA SUBSCRIBER PRICE -4.16

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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=> file caold SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 0.42 690.05 FULL ESTIMATED COST TOTAL SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION 0.00 -4.16 CA SUBSCRIBER PRICE

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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FILE 'REGISTRY' ENTERED AT 12:29:18 ON 17 MAY 2004
L1 STRUCTURE UPLOADED

L2 50 S L1

L3 1375 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 12:37:16 ON 17 MAY 2004 L4 776 S L3

FILE 'REGISTRY' ENTERED AT 12:37:21 ON 17 MAY 2004

L5 STRUCTURE UPLOADED
L6 STRUCTURE UPLOADED
L7 STRUCTURE UPLOADED

L8 0 S L7

L9 0 S L7 FULL

L10 STRUCTURE UPLOADED

L11 0 S L10

L12 0 S L10 FULL

L13 STRUCTURE UPLOADED

L14 0 S L13

L15 6 S L13 FULL

FILE 'HCAPLUS' ENTERED AT 13:04:21 ON 17 MAY 2004

L16 6 S L15

L17 0 S L16 AND PRIESTLEY, E?/AU

L18 0 S L15 AND DECICCO, C?/AU

L19 0 S L15 AND HUDYMA, T?/AU

FILE 'HCAPLUS' ENTERED AT 13:05:52 ON 17 MAY 2004

FILE 'CAOLD' ENTERED AT 13:07:24 ON 17 MAY 2004

FILE 'CAOLD' ENTERED AT 13:07:26 ON 17 MAY 2004

=> s 115

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ring bonds :
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normalized bonds :
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                                        15-16
                  12-13
isolated ring systems :
    containing 1 : 11 :
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G1:CH, N

chain nodes :

G2:Cy, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 40:Atom 41:Atom 42:Atom 43:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 52:CLASS 53:CLASS 54:CLASS 57:CLASS 58:Atom

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ring nodes :
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chain bonds :
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                                                                    56-60
ring bonds :
    1-2 1-6 2-3 3-4
                         4 - 5
                              5-6 5-7
                                         6-9
                                              7-8 8-9
                                                         11-12
                                                                11-16 12-13
                  15-16
                          22-23
                                22-26
                                         23-24
    13-14
           14-15
                                                24-25
                                                        25-26
                                                               28-29
                                                                      28-32
    29-30
           30 - 31
                   31-32
                          34-35
                                 34 - 38
                                         35-36
                                                36-37
                                                        37-38
                                                               40-41
                                                                      40 - 43
    41-56
           42-43
                   42-56
                          45-46
                                 45-49
                                         46-47
                                                47-48
                                                        48-49
exact/norm bonds :
                                         5 - 7
    1-2 1-6 2-3
                   3 – 4
                         3-58 4-5 5-6
                                               6-9 7-8 8-9
                                                               8-12
                                                                     15 - 17
    17-59
          19-20
                  20-21
                          22-23
                                 22-26
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                                                               28-29
                                                                      28-32
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                   31 - 32
                          34 - 35
                                 34-38
                                         35-36
                                                36-37
                                                        37-38
                                                               40-41
                                                                      40-43
           42-43
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                          45-46
                                 45-49
    41-56
                                         46-47
                                                47-48
                                                        47-61
                                                               48-49
                                                                      52 - 53
    53-54
           56-60
normalized bonds :
          11-16 12-13
    11-12
                          13-14
                                14-15
                                         15-16
isolated ring systems :
    containing 1 : 11 :
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G1:CH, N

G2: [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 40:Atom 41:Atom 42:Atom 43:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 52:CLASS 53:CLASS 54:CLASS 56:Atom 58:CLASS 59:CLASS 60:CLASS 61:CLASS

* * * * *	* * *	* *	* Welcome to STN International * * * * * * * * *	
NEWS 1			Web Page URLs for STN Seminar Schedule - N. America	
NEWS 2	T 20 3.T	2.7	"Ask CAS" for self-help around the clock	1
NEWS 3	JAN	21	Source of Registration (SR) information in REGISTRY updated and searchable	1
NEWS 4	JAN	27	A new search aid, the Company Name Thesaurus, available in CA/CAplus	
NEWS 5	FEB	05	German (DE) application and patent publication number formatchanges	at
NEWS 6	MAR	03	MEDLINE and LMEDLINE reloaded	
NEWS 7	MAR		MEDLINE file segment of TOXCENTER reloaded	
NEWS 8	MAR		FRANCEPAT now available on STN	
NEWS 9	MAR	29	Pharmaceutical Substances (PS) now available on STN	
NEWS 10	MAR	29	WPIFV now available on STN	
NEWS 11	MAR	29	New monthly current-awareness alert (SDI) frequency in RAPF	RA.
NEWS 12	APR	26	PROMT: New display field available	
NEWS 13	APR	26	<pre>IFIPAT/IFIUDB/IFICDB: New super search and display field available</pre>	
NEWS 14	APR	26		
NEWS 15			NLDB: New search and display fields available	
NEWS 16			PROUSDDR now available on STN	
NEWS 17	_			
	1		and June 2004	
NEWS 18	May	12		
NEWS 19	•			RY
NEWS 20	_			
NEWS EXF	RESS		RCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),	
			CINIOSH VERSION IS V6.0C(ENG) AND V6.00C(OF), CURRENT DISCOVER FILE IS DATED 26 APRIL 2004	
MENTO HOL	TD C		O Operating Hours Plus Help Desk Availability	
NEWS HOU			n operating hours Plus help besk Availability neral Internet Information	
NEWS INT			lcome Banner and News Items	
NEWS LOC			rect Dial and Telecommunication Network Access to STN	
NEWS PHO			S World Wide Web Site (general information)	
NEWS WWW	-			
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			for software development or design or implementation	
			ateways or other similar uses is prohibited and may	
result	in lo	oss (of user privileges and other penalties.	
* * * *	* * *	* *	* * * * * STN Columbus * * * * * * * * * * * * *	
FILE 'HOM	1E' E1	ITER:	ED AT 14:43:44 ON 17 MAY 2004	
=> file r	eg			
COST IN U		OOLL	ARS SINCE FILE TOTAL	
			ENTRY SESSION	
FULL ESTI	MATE	CO.	0.21 0.21	

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1 DICTIONARY FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

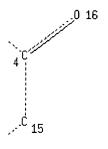
Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L1 STRUCTURE UPLOADED

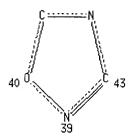
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41 4241 Page 1-A Cy 55

Page 1-C



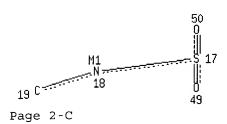
Page 1-D



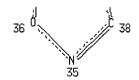
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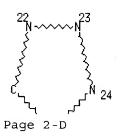


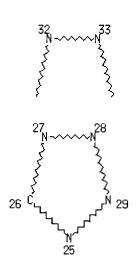
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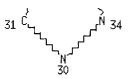
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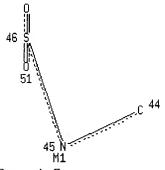








Page 3-D



Page 4-C VAR G1=53/54

VAR G2=55/17/21/25/33/38/43/44

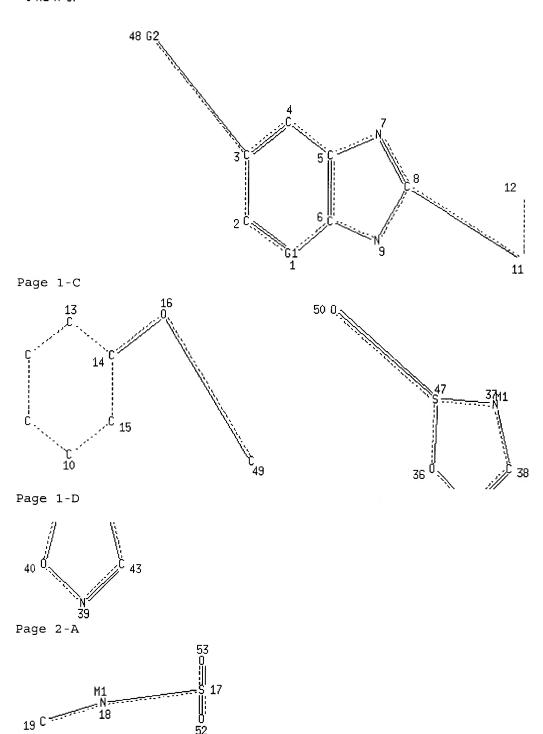
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NSPEC	IS	R	AΤ	5	
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NSPEC	IS	R	AT	9	
NSPEC	IS	R	AΤ	10	
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NSPEC	IS	R	AT	13	
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NSPEC	IS	R	AT	15	
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NSPEC	IS	С	AT	17	
NSPEC	IS	С	AT	18	
NSPEC	IS	C	AT	19	
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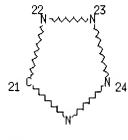
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               AT 45
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               AT 46
              AT 46
AT 47
AT 48
AT 49
NSPEC IS C
NSPEC
       IS R
      IS C
NSPEC
NSPEC IS C
               AT 50
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               AT 51
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MLEVEL IS CLASS AT 16 17 18 19 44 45 46 49 50 51 52 55
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 1 11
NUMBER OF NODES IS 55
STEREO ATTRIBUTES: NONE
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SAMPLE SCREEN SEARCH COMPLETED - 617 TO ITERATE
100.0% PROCESSED
                   617 ITERATIONS
                                                          34 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS:
                     10850 TO 13830
PROJECTED ANSWERS:
                           331 TO
                                      1029
L2
            34 SEA SSS SAM L1
=>
       STRUCTURE UPLOADED
L3
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L3 HAS NO ANSWERS
L3
3
51 0
              STR
Page 1-A
56
Page 1-B
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C M1 N 57

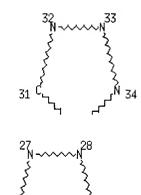
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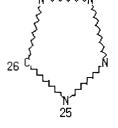


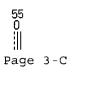




Page 2-D



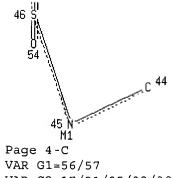




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29 Page 3-D



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VAR G2=			3/38/	/43/4
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HCOUNT	IS	Ml	AT	37
HCOUNT	IS	M1	AT	42
HCOUNT	IS	M1	AT	45
HCOUNT	IS		AT	56
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AΤ	5
NSPEC	IS		AT	6
NSPEC	IS		AT	7
NSPEC	IS		AT	8
NSPEC	IS	R	AT	9
NSPEC	IS		AT	10
NSPEC	IS		AT	11
NSPEC	IS		AT	12
NSPEC	IS		AT	13
NSPEC				
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	IS		AT	16
NSPEC	IS		AΤ	
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NSPEC	IS		AT	19
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NSPEC	IS	R	AΤ	33
NSPEC	IS	R	AT	34
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NSPEC	IS	R	AT	40
NSPEC	IS	R	AT	41
20				

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AT 42
NSPEC IS R

        NSPEC
        IS R
        AT
        42

        NSPEC
        IS R
        AT
        43

        NSPEC
        IS C
        AT
        44

        NSPEC
        IS C
        AT
        45

        NSPEC
        IS C
        AT
        46

        NSPEC
        IS C
        AT
        47

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        IS C
        AT
        49

        NSPEC
        IS C
        AT
        50

        NSPEC
        IS C
        AT
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        AT
        53

        NSPEC
        IS C
        AT
        54

NSPEC IS C
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DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 16 17 18 19 44 45 46 49 50 51 52 53 54 55
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 1 11
NUMBER OF NODES IS 57
STEREO ATTRIBUTES: NONE
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SAMPLE SEARCH INITIATED 14:49:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE
100.0% PROCESSED
                             13 ITERATIONS
                                                                                               10 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                                    BATCH **COMPLETE**
                                                44 TO 476
PROJECTED ITERATIONS:
PROJECTED ANSWERS:
                                                11 TO
                                                                389
L4
                   10 SEA SSS SAM L3
=> s 13 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:49:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 232 TO ITERATE
100.0% PROCESSED
                                232 ITERATIONS
                                                                                           161 ANSWERS
SEARCH TIME: 00.00.01
L5
               161 SEA SSS FUL L3
=> file hcaplus
COST IN U.S. DOLLARS
                                                                           SINCE FILE TOTAL
                                                                                 ENTRY SESSION
158.78 158.99
FULL ESTIMATED COST
FILE 'HCAPLUS' ENTERED AT 14:49:12 ON 17 MAY 2004
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```

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FILE COVERS 1907 - 17 May 2004 VOL 140 ISS 21 FILE LAST UPDATED: 16 May 2004 (20040516/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6

3 L5

=> d 16, ibib abs fhitstr, 1-3

L6 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References Text

ACCESSION NUMBER: 2003:261620 HCAPLUS

DOCUMENT NUMBER: 138:287673

TITLE: Preparation of phenylbenzimidazole compounds useful

for treating hepatitis C virus

INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,

Thomas W.; Zheng, Xiaofan

Bristol-Myers Squibb Company, USA PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO.
                    KIND DATE
                                         APPLICATION NO. DATE
                    _ _ _ _
                          -----
                                         -----
                    A2
    WO 2003026587
                                         WO 2002-US30989 20020926
                           20030403
    WO 2003026587
                    A3
                           20031106
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
            CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
            PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
            NE, SN, TD, TG
                  A1
                          20030717
    US 2003134853
                                         US 2002-259041
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    US 2004067976
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                          20040408
                                         US 2003-648873
                                                          20030827
PRIORITY APPLN. INFO.:
                                      US 2001-324874P P 20010926
                                      US 2002-259041 B1 20020926
OTHER SOURCE(S):
                     MARPAT 138:287673
```

GT

$$R1$$
 Q
 N
 $R3$
 $C1$

AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 µM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 503857-56-5 HCAPLUS

CN Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 503857-55-4 CMF C40 H41 N7 O5 S

CM 2

 $\frac{76-05-1}{CMF}$ C2 H F3 O2

PRIORITY APPLN. INFO.: JP 2001-193786 A 20010626

<u>JP 2001-351537</u> A 20011116

WO 2002-JP6405 W 20020626

OTHER SOURCE(S): MARPAT 138:66657

Ι

GI

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

IT 480462-18-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 480462-18-8 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, 4'-chloro-2-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]-3-fluorophenoxy]methyl]-N,N-dimethyl-(9CI) (CA INDEX NAME)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold COST IN U.S. DOLLARS	SINCE FILE	TOTAL SESSION
FULL ESTIMATED COST	18.99	177.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.08	-2.08

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

=> d his

L1

(FILE 'HOME' ENTERED AT 14:43:44 ON 17 MAY 2004)

FILE 'REGISTRY' ENTERED AT 14:43:56 ON 17 MAY 2004

STRUCTURE UPLOADED

L2 34 S L1

L3 STRUCTURE UPLOADED

L4 10 S L3

L5 161 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 14:49:12 ON 17 MAY 2004 L6 3 S L5

FILE 'CAOLD' ENTERED AT 14:50:21 ON 17 MAY 2004

=> s 15

L7 0 L5

=>

* * * * * * * * Welcome to STN International Web Page URLs for STN Seminar Schedule - N. America NEWS NEWS 2 "Ask CAS" for self-help around the clock NEWS JAN 27 Source of Registration (SR) information in REGISTRY updated 3 and searchable NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAplus NEWS 5 FEB 05 German (DE) application and patent publication number format changes NEWS 6 MAR 03 MEDLINE and LMEDLINE reloaded NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded NEWS 8 MAR 03 FRANCEPAT now available on STN NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN NEWS 10 MAR 29 WPIFV now available on STN NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA NEWS 12 APR 26 PROMT: New display field available NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field available NEWS 14 APR 26 LITALERT now available on STN NEWS 15 APR 27 NLDB: New search and display fields available NEWS 16 May 10 PROUSDDR now available on STN NEWS 17 May 19 PROUSDDR: One FREE connect hour, per account, in both May and June 2004 NEWS 18 May 12 EXTEND option available in structure searching NEWS 19 May 12 Polymer links for the POLYLINK command completed in REGISTRY NEWS 20 May 17 FRFULL now available on STN NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004 STN Operating Hours Plus Help Desk Availability NEWS HOURS NEWS INTER General Internet Information Welcome Banner and News Items NEWS LOGIN Direct Dial and Telecommunication Network Access to STN NEWS PHONE NEWS WWW CAS World Wide Web Site (general information) Enter NEWS followed by the item number or name to see news on that specific topic.

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SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

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0.21

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STRUCTURE FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1 DICTIONARY FILE UPDATES: 16 MAY 2004 HIGHEST RN 682330-24-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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FULL ESTIMATED COST

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* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *

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COST IN U.S. DOLLARS

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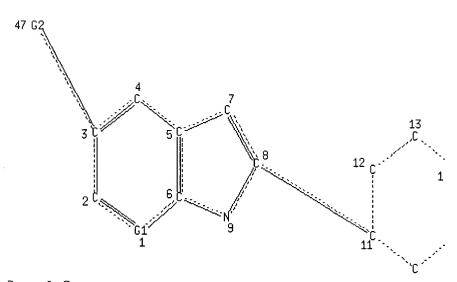
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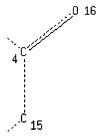
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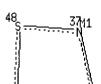
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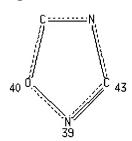


Page 1-C

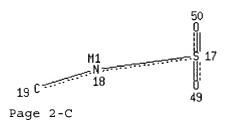




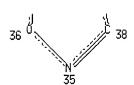
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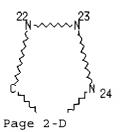


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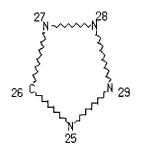










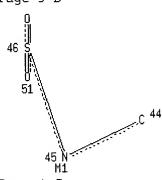


52 Page 3-C





Page 3-D



Page 4-C VAR G1=53/54

VAR G2=55/17/21/25/33/38/43/44

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DEFAULT ECLEVEL IS LIMITED
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SAMPLE SEARCH INITIATED 14:06:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
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                                                           3 ANSWERS
 53.9% PROCESSED
                  1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                              **COMPLETE**
                      BATCH
PROJECTED ITERATIONS:
                      34498 TO 39662
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PROJECTED ANSWERS:

3 TO 252

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100.0% PROCESSED 36521 ITERATIONS

26 ANSWERS

SEARCH TIME: 00.00.02

L3 26 SEA SSS FUL L1

=> file hcaplus
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SINCE FILE TOTAL ENTRY SESSION 170.54 170.75

FULL ESTIMATED COST

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=> s 13

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=> d 14, ibib abs fhitstr, 1-7

L4 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

2001:787194 HCAPLUS

DOCUMENT NUMBER:

136:69709

TITLE:
AUTHOR(S):

Solid-Phase Synthesis of 2,3,5-Trisubstituted Indoles

Wu, Tom Y. H.; Ding, Sheng; Gray, Nathanael S.;

Schultz, Peter G.

CORPORATE SOURCE:

Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La

Jolla, CA, 92037, USA

SOURCE:

Organic Letters (2001), 3(24), 3827-3830

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

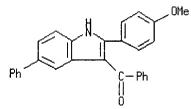
AB 2,3,5-Trisubstituted indoles are synthesized in three steps starting from resin-bound 4-bromo-2-iodoaniline. The substituent on the 2-position of the indole is introduced by a palladium-mediated coupling of the iodoaniline with terminal alkynes followed by intramol. cyclization to form the indole core. Acylation with an acid chloride in the presence of AlCl3 catalyst introduces the substituent at the 3-position of the indole. The indole C-5 position is then diversified either by Sonagashira or Suzuki couplings with the bromide. Finally, indole N-1 can be modified by post-cleavage methylation.

IT 385370-44-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of 2,3,5-trisubstituted indoles)

RN 385370-44-5 HCAPLUS

CN Methanone, [2-(4-methoxyphenyl)-5-phenyl-1H-indol-3-yl]phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

16

Full Citing Text References

ACCESSION NUMBER: 1997:238314 HCAPLUS

DOCUMENT NUMBER: 126:225300

TITLE: Preparation of benzazoles as radioprotectors.

INVENTOR(S): Martin, Roger Francis; Kelly, David Patterson; White,

Johnathon Michael

PATENT ASSIGNEE(S): Peter Maccallum Cancer Institute, Australia

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT	NO.		KI	ND	DATE			A.	PPLI	CATI	ON N	٥.	DATE			
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WO 970	<u> 1776</u>		A	1	1997	0213		W	0 19	96-A	U467		1996	0726		
W:	AL,	AM,	AT,	ΑU,	ΑZ,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	DK,
	EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LK,	LR,
	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,
	SD,	SE														
RW	: KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM			
CA 222	3044		A	A	1997	0213		C	A 19	96-2	2280	44	1996	0726		
AU 966	5096		A	1	1997	0226		A	J 19	96-6	5096		1996	0726		
AU 717	249		В	2	2000	0323										

EP 857067 Α1 19980812 EP 1996-924709 19960726 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI JP 2000501697 T2 20000215 JP 1997-507005 19960726 US 6194414 В1 20010227 US 1998-313 19980428 US 2000-637903 US 6548505 B1 20030415 20000814 A 19950728 PRIORITY APPLN. INFO.: AU 1995-4492 WO 1996-AU467 W 19960726 US 1998-313 A2 19980428 OTHER SOURCE(S):

MARPAT 126:225300

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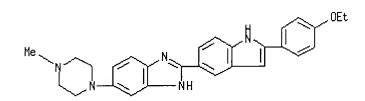
AΒ Use of title compds. [I; X = (substituted) aminoalkyl, alkylene, interactive group; Y, Z = N, O, S CR; R = H, (substituted) alkyl, alkenyl; dotted line = double bond unless the attached Y or Z group = O or S in which case it is a single bond; d R1-R11 = H, a sterically hindering group and an electron donating group; any 2 of R1 R11, Y, Z, NH and R may form a (substituted) ring which may contain heteroatoms, provided that ≥1 of R1-R11 = electron donating group and that when X = NMe, Y and Z = N and R1, R2, and R4-R11 = H, then R3 \neq OH or OCH2Me] as radioprotectants, is claimed. Thus, 2-amino-4-(1-piperidinyl)amine and 4-dimethylamino-1-[5-(iminoethoxy)methylbenzimidazol-2-yl]benzene hydrochloride (prepn. given) were refluxed 3 h in HOAc/EtOH to give 4-dimethylamino-1-[5-[5-(piperidin-1-yl)benzimidazol-2-yl]benzimidazol-2-yl]benzene. The latter at 17 μM in cell culture studies gave a protection factor of 2.7-2.8.

IT 188247-18-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of benzazoles as radioprotectors)

RN 188247-18-9 HCAPLUS

1H-Benzimidazole, 2-[2-(4-ethoxyphenyl)-1H-indol-5-yl]-5-(4-methyl-1-CNpiperazinyl) - (9CI) (CA INDEX NAME)



ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing Full Text References ACCESSION NUMBER:

1995:647297 HCAPLUS

DOCUMENT NUMBER: 123:143666

TITLE: Synthesis of 5- and 6-membered heterocycles by a strategy combining SNAr and SRN1 reactions

AUTHOR (S): Beugelmans, Rene; Chbani, Mohamed

CORPORATE SOURCE: Institut Chimie Substances Naturelles, CNRS,

Gif-sur-Yvette, 91198, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1995),

132(3), 306-13

CODEN: BSCFAS; ISSN: 0037-8968

PUBLISHER: Elsevier DOCUMENT TYPE: Journal French LANGUAGE:

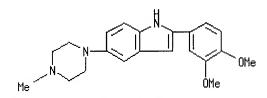
The SRN1 mechanism is compatible with many substituents on the benzenic substrate and allows SRN1 reactions to be combined with SNAr reactions in a strategy which brings together their corresponding synthetic advantages. Thus, compds. contg. benzene fused to 5- or 6-membered heterocycles contg. N (indoles), N and P (benzazaphospholes) and N and S (benzothiazines) are readily obtained.

IT 166818-63-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 5- and 6-membered heterocycles by a strategy combining SNAr and SRN1 reactions)

166818-63-9 HCAPLUS RN

1H-Indole, 2-(3,4-dimethoxyphenyl)-5-(4-methyl-1-piperazinyl)- (9CI) (CA CNINDEX NAME)



ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN L4

Citing Full Text References

1991:679809 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 115:279809

TITLE: Preparation of 2-phenylindole derivatives as

lipoxygenase inhibitors

Suzuki, Yasushi; Hasegawa, Yukio; Sato, Michitaka; INVENTOR (S):

Yamamoto, Norio; Hasumi, Koichi; Shidara, Kazuhiro;

Miyasaka, Katsuhiko; Kenjo, Takashi; Miyazawa,

Katsuhiko; Et, Al.

Teikoku Hormone Mfg. Co., Ltd., Japan PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 16 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
JP 03188064	A2	19910816	JP 1989-326634	19891216	
JP 2894617	B2	19990524			
PRIORITY APPLN. INFO.	:		JP 1989-326634	19891216	

OTHER SOURCE(S): MARPAT 115:279809

GT

$$R^2$$
 R^3
 R^4
 R^5
 R^5
 R^1
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 R^1
 R^5
 R^6
 R^6

2-Phenylindole derivs. [I; R1 = H, alkyl; R2-R4 = H, halo, alkyl, alkoxy, etc.; R5 = H, alkyl], effective lipoxygenase and cyclooxygenase inhibitors, are prepd. Refluxing a mixt. of 60 g ketone II and 55 g 4-AcnHC6H4NHNH2.HCl in Me2CHOH gave 78 g I (R1 = Me, R2 = R3 = R5 = H, R4 = 5-AcnH), which showed 82% inhibition of 5-HETE at 10 μ M. Also prepd. and tested were 25 addnl. I.

IT 137614-73-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as lipoxygenase inhibitor)

RN 137614-73-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[2-[3-(1,1-dimethylethyl)-4-hydroxy-5-methylphenyl]-3-methyl-1H-indol-5-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1990:571973 HCAPLUS

DOCUMENT NUMBER: 113:171973

TITLE: Nonsteroidal cardiotonics. 3. New

4,5-dihydro-6-(1H-indol-5-yl)pyridazin-3(2H)-ones and related compounds with positive inotropic activities

AUTHOR(S): Mertens, Alfred; Friebe, Walter Gunar;

Mueller-Beckmann, Bernd; Kampe, Wolfgang; Kling,

Lothar; Von der Saal, Wolfgang

CORPORATE SOURCE: Dep. Chem., Boehringer Mannheim G.m.b.H., Mannheim,

6800, Germany

SOURCE: Journal of Medicinal Chemistry (1990), 33(10), 2870-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:171973

GΙ

A series of substituted indolyldihydropyridazinones I (R = Ph, CO2Et, 3-, AΒ 4-pyridyl, 4-MeC6H4; R1 = H, Me, Et, CHMe2; R2 = H, Me) and related compds. were synthesized and evaluated for pos. inotropic activity. rats, most of these indole derivs. produced a dose-related increase in myocardial contractility with little effect on heart rate and blood pressure. I (R = 4-pyridy1, R1 = H; R2 = Me), (II, BM 50.0430), wasfurther investigated in cats. The increase in contractility in this animal model was not mediated via stimulation of β -adrenergic receptors. After oral administration of 1 mg/kg to conscious dogs, II and pimobendan were still active after 6.5 h. However, the cardiotonic effect of II was at least 2-fold that of pimobendan after this period of time. The structural requirements for optimal cardiotonic activity within this class of indole derivs. are a heterocyclic arom. ring in position 2, a hydrogen or a Me group in position 3 and a dihydropyridazinone ring system in position 5 of the indole.

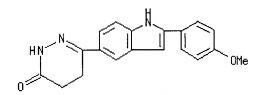
IT 129593-70-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and inotropic activity of)

RN 129593-70-0 HCAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-6-[2-(4-methoxyphenyl)-1H-indol-5-yl]-(9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 1984:209577 HCAPLUS

DOCUMENT NUMBER: 100:209577

TITLE: Syntheses of antimicrobial biscationic

2-(phenoxyphenyl)indoles and -1-benzofurans
AUTHOR(S): Dann, Otto; Ruff, Juergen; Wolff, Hans Peter;

Griessmeier, Helmut

CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ.

Erlangen-Nurnberg, Erlangen, D-8520, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1984), (3), 409-25

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 100:209577

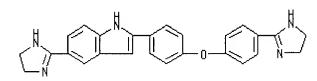
GΙ

AB Ten 2-(phenoxyphenyl)indoles and 4 2-(phenoxyphenyl)-1-benzofurans with terminal amidinium or imidazolinium groups, e.g. I and II, were prepd. as antimicrobials. Thus, 4,2-Br(O2N)C6H3CH2COC6H4(OC6H4Br-p)-p, prepd. from 4,3-Br(O2N)C6H3CH2CO2H and p-BrC6H4OPh, underwent reductive cyclization followed by reaction with CuCN to give the indole III which was aminated with NH3 to give I.

IT 90178-91-9P

RN 90178-91-9 HCAPLUS

CN 1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-imidazol-2-yl)phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1983:569063 HCAPLUS

DOCUMENT NUMBER: 99:169063

TITLE: Inhibitory activity of diarylamidine derivatives on

murine leukemia L1210 cell growth

AUTHOR(S): Balzarini, Jan; De Clercq, Erik; Dann, Otto

CORPORATE SOURCE: Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain,

B-3000, Belg.

SOURCE: Investigational New Drugs (1983), 1(2), 103-15

CODEN: INNDDK; ISSN: 0167-6997

DOCUMENT TYPE: Journal

LANGUAGE: English

GΙ



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Weinheim [Ger.] Verlag Chemie, 1979-1994.

Notes:

Summaries in English.

ISSN:

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Bioorganic chemistry -- Periodicals.

Chemistry, Organic -- Periodicals.

v.: ill.; 24 cm.

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Main run: Vol. 691, No. 1 - Vol. 1994, No. 12 (Jan 1966 - Dec 1994)

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AB A series of 96 diarylamidine and diarylamidazoline derivs., mostly I (X =NH, O, S, SO2, CH2; Y = CH, CNH2, N, etc.; R1 and R2 = amidino, imidazolino, etc.; Z = CH:CH, PhO, CONH, NH, etc; n = 0 or 1), II (R1 and R2 = amidino or imidazolino; Z = CH:CH, NHN:N, etc.), III (X = O, S, or NH; Y = CH, CMe, N; R1 and R2 = amidino or imidazolino), and IV (X = NH; Y = CH; Z = CH:CH; R1 and R2 = imidazolino; n = 0 or 1), were tested for antitumor activity against murine leukemia L1210 cells. Structure-function anal. revealed that the antitumor activity of the diarylamidines depended on the planarity of the mol., the presence of amidino or, preferably, imidazolino groups or both aryl moieties, the nature of the bridge connecting the 2 aryl moieties, and the nature of the aryl moieties (preferably benzofuren or benzo[b]thiophene. Thus, (6-(2-imidazolin-2-yl)-2-[4-(2-imidazolin-2-yl)phenyl]benzo[b]thiophene (I; X = S; Y = CH; R1 = R2 = imidazolino; n = 0) [73819-21-3] was the most potent inhibitor of L1210 cell growth. The inhibitory effects of diarylamidines on L1210 cell proliferation may at least partly involve an inhibition of DNA synthesis. 2,2'-Vinylenedi-1-benzofuran-5-carboxamidine (III; X = O; Y = CH; Z = CH:CH; R1 = R2 = amidino) [65426-90-6] exhibited potent antitumor activity in vitro and in vivo in L1210-inoculated mice.

IT 87559-26-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(neoplasm inhibitory activity of, structure in relation to)

RN 87559-26-0 HCAPLUS

1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-imidazol-2-yl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

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FILE 'REGISTRY' ENTERED AT 13:43:42 ON 17 MAY 2004

L1 STRUCTURE UPLOADED

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L3 26 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:06:23 ON 17 MAY 2004

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L7 0 L3 AND HUDYMA, T?/AU

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L4 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2001:787194 HCAPLUS

DOCUMENT NUMBER: 136:69709

TITLE: Solid-Phase Synthesis of 2,3,5-Trisubstituted Indoles

AUTHOR(S): Wu, Tom Y. H.; Ding, Sheng; Gray, Nathanael S.;

Schultz, Peter G.

CORPORATE SOURCE: Department of Chemistry and the Skaggs Institute for

Chemical Biology, The Scripps Research Institute, La

Jolla, CA, 92037, USA

SOURCE: Organic Letters (2001), 3(24), 3827-3830

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB 2,3,5-Trisubstituted indoles are synthesized in three steps starting from resin-bound 4-bromo-2-iodoaniline. The substituent on the 2-position of the indole is introduced by a palladium-mediated coupling of the iodoaniline with terminal alkynes followed by intramol. cyclization to form the indole core. Acylation with an acid chloride in the presence of AlCl3 catalyst introduces the substituent at the 3-position of the indole. The indole C-5 position is then diversified either by Sonagashira or Suzuki couplings with the bromide. Finally, indole N-1 can be modified by post-cleavage methylation.

IT 385370-44-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of 2,3,5-trisubstituted indoles)

RN <u>385370-44-5</u> HCAPLUS

CN Methanone, [2-(4-methoxyphenyl)-5-phenyl-1H-indol-3-yl]phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text References

ACCESSION NUMBER: 1997:238314 HCAPLUS

DOCUMENT NUMBER: 126:225300

TITLE: Preparation of benzazoles as radioprotectors.

INVENTOR(S): Martin, Roger Francis; Kelly, David Patterson; White,

Johnathon Michael

PATENT ASSIGNEE(S): Peter Maccallum Cancer Institute, Australia

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

	PAT	CENT 1	NO.		KI	ND .	D DATE APPLICATION NO.				ο.	DATE						
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	WO	9704	776		Α	1	1997	0213		W	O 19	96-A	U467		1996	0726		
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			LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,
			SD,															
		RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
			ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM			
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	AU	9665	096		A	1	1997	0226		A	J 19	96-6	5096		1996	0726		
	AU	7172	49		B	2	2000	0323										
	EP	8570	67		A	1	1998	0812		E	P 19	96-92	2470	9	1996	0726		
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	FI														
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	US	6194	114		B	1 :	2001	0227		<u>U</u> .	3 19	98-3	13		1998	0428		
	US	6548	505		B	1 :	2003	0415		<u>U</u> :	3 20	00-63	3790	3	2000	0814		
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OTHER SOURCE(S): MARPAT 126:225300

GΙ

Use of title compds. [I; X = (substituted) aminoalkyl, alkylene, AB interactive group; Y, Z = N, O, S CR; R = H, (substituted) alkyl, alkenyl; dotted line = double bond unless the attached Y or Z group = O or S in which case it is a single bond; d R1-R11 = H, a sterically hindering group and an electron donating group; any 2 of R1 R11, Y, Z, NH and R may form a (substituted) ring which may contain heteroatoms, provided that ≥1

of R1-R11 = electron donating group and that when X = NMe, Y and Z = N and R1, R2, and R4-R11 = H, then R3 \neq OH or OCH2Me] as radioprotectants, is claimed. Thus, 2-amino-4-(1-piperidinyl)amine and 4-dimethylamino-1-[5-(iminoethoxy)methylbenzimidazol-2-yl]benzene hydrochloride (prepn. given) were refluxed 3 h in HOAc/EtOH to give 4-dimethylamino-1-[5-[5-(piperidin-1-yl)benzimidazol-2-yl]benzimidazol-2-yl]benzene. The latter at 17 μM in cell culture studies gave a protection factor of 2.7-2.8.

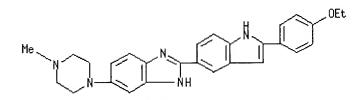
IT 188247-18-9P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of benzazoles as radioprotectors)

RN 188247-18-9 HCAPLUS

1H-Benzimidazole, 2-[2-(4-ethoxyphenyl)-1H-indol-5-yl]-5-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1995:647297 HCAPLUS

DOCUMENT NUMBER: 123:143666

TITLE: Synthesis of 5- and 6-membered heterocycles by a

strategy combining SNAr and SRN1 reactions

AUTHOR(S): Beugelmans, Rene; Chbani, Mohamed

CORPORATE SOURCE: Institut Chimie Substances Naturelles, CNRS,

Gif-sur-Yvette, 91198, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1995),

132(3), 306-13

CODEN: BSCFAS; ISSN: 0037-8968

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: French

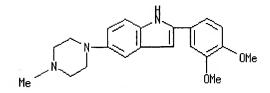
The SRN1 mechanism is compatible with many substituents on the benzenic substrate and allows SRN1 reactions to be combined with SNAr reactions in a strategy which brings together their corresponding synthetic advantages. Thus, compds. contg. benzene fused to 5- or 6-membered heterocycles contg. N (indoles), N and P (benzazaphospholes) and N and S (benzothiazines) are readily obtained.

IT 166818-63-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 5- and 6-membered heterocycles by a strategy combining SNAr and SRN1 reactions)

RN 166818-63-9 HCAPLUS

CN 1H-Indole, 2-(3,4-dimethoxyphenyl)-5-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References

ACCESSION NUMBER:

1991:679809 HCAPLUS

DOCUMENT NUMBER:

115:279809

TITLE:

Preparation of 2-phenylindole derivatives as

lipoxygenase inhibitors

INVENTOR(S):

Suzuki, Yasushi; Hasegawa, Yukio; Sato, Michitaka; Yamamoto, Norio; Hasumi, Koichi; Shidara, Kazuhiro;

Miyasaka, Katsuhiko; Kenjo, Takashi; Miyazawa,

Katsuhiko; Et, Al.

PATENT ASSIGNEE(S):

Teikoku Hormone Mfg. Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO.	DATE		
JP 03188064	A2	19910816		JP 1989-326634	19891216		
JP 2894617	B2	19990524					
PRIORITY APPLN. INFO.	:		JP	1989-326634	19891216		
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OTHER SOURCE(S):

MARPAT 115:279809

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2-Phenylindole derivs. [I; R1 = H, alkyl; R2-R4 = H, halo, alkyl, alkoxy, AB etc.; R5 = H, alkyl], effective lipoxygenase and cyclooxygenase inhibitors, are prepd. Refluxing a mixt. of 60 g ketone II and 55 g 4-AcNHC6H4NHNH2.HC1 in Me2CHOH gave 78 g I (R1 = Me, R2 = R3 = R5 = H, R4 = 5-AcNH), which showed 82% inhibition of 5-HETE at 10 μM . Also prepd. and tested were 25 addnl. I.

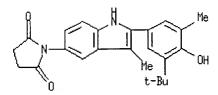
IT 137614-73-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as lipoxygenase inhibitor)

RN 137614-73-4 HCAPLUS

2,5-Pyrrolidinedione, 1-[2-[3-(1,1-dimethylethyl)-4-hydroxy-5-CN methylphenyl]-3-methyl-1H-indol-5-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1990:571973 HCAPLUS

DOCUMENT NUMBER: 113:171973

TITLE: Nonsteroidal cardiotonics. 3. New

4,5-dihydro-6-(1H-indol-5-yl)pyridazin-3(2H)-ones and related compounds with positive inotropic activities

AUTHOR(S): Mertens, Alfred; Friebe, Walter Gunar;

Mueller-Beckmann, Bernd; Kampe, Wolfgang; Kling,

Lothar; Von der Saal, Wolfgang

CORPORATE SOURCE: Dep. Chem., Boehringer Mannheim G.m.b.H., Mannheim,

6800, Germany

SOURCE: Journal of Medicinal Chemistry (1990), 33(10), 2870-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:171973

GΙ

A series of substituted indolyldihydropyridazinones I (R = Ph, CO2Et, 3-, AB 4-pyridyl, 4-MeC6H4; R1 = H, Me, Et, CHMe2; R2 = H, Me) and related compds. were synthesized and evaluated for pos. inotropic activity. In rats, most of these indole derivs. produced a dose-related increase in myocardial contractility with little effect on heart rate and blood pressure. I (R = 4-pyridyl, R1 = H; R2 = Me), (II, BM 50.0430), wasfurther investigated in cats. The increase in contractility in this animal model was not mediated via stimulation of $\beta\text{-adrenergic}$ receptors. After oral administration of 1 mg/kg to conscious dogs, II and pimobendan were still active after 6.5 h. However, the cardiotonic effect of II was at least 2-fold that of pimobendan after this period of time. The structural requirements for optimal cardiotonic activity within this class of indole derivs. are a heterocyclic arom. ring in position 2, a hydrogen or a Me group in position 3 and a dihydropyridazinone ring system in position 5 of the indole.

IT 129593-70-0P

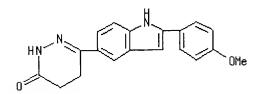
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and inotropic activity of)

RN 129593-70-0 HCAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-6-[2-(4-methoxyphenyl)-1H-indol-5-yl]-

(9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1984:209577 HCAPLUS

DOCUMENT NUMBER: 100:209577

TITLE: Syntheses of antimicrobial biscationic

2-(phenoxyphenyl)indoles and -1-benzofurans

AUTHOR(S): Dann, Otto; Ruff, Juergen; Wolff, Hans Peter;

Griessmeier, Helmut

CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ.

Erlangen-Nurnberg, Erlangen, D-8520, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1984), (3), 409-25

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE:

LANGUAGE:

DANGUAGE.

OTHER SOURCE(S):

Journal German

CASREACT 100:209577

GI

Ten 2-(phenoxyphenyl)indoles and 4 2-(phenoxyphenyl)-1-benzofurans with terminal amidinium or imidazolinium groups, e.g. I and II, were prepd. as antimicrobials. Thus, 4,2-Br(O2N)C6H3CH2COC6H4(OC6H4Br-p)-p, prepd. from 4,3-Br(O2N)C6H3CH2CO2H and p-BrC6H4OPh, underwent reductive cyclization followed by reaction with CuCN to give the indole III which was aminated with NH3 to give I.

IT 90178-91-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 90178-91-9 HCAPLUS

CN 1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-imidazol-2-yl)phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

2 HC1

L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 1983:569063 HCAPLUS

DOCUMENT NUMBER: 99:169063

TITLE: Inhibitory activity of diarylamidine derivatives on

murine leukemia L1210 cell growth

AUTHOR(S): Balzarini, Jan; De Clercq, Erik; Dann, Otto

CORPORATE SOURCE: Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain,

B-3000, Belg.

SOURCE: Investigational New Drugs (1983), 1(2), 103-15

CODEN: INNDDK; ISSN: 0167-6997

DOCUMENT TYPE: Journal

LANGUAGE: English

GΙ

A series of 96 diarylamidine and diarylamidazoline derivs., mostly I (X =AB NH, O, S, SO2, CH2; Y = CH, CNH2, N, etc.; R1 and R2 = amidino, imidazolino, etc.; Z = CH:CH, PhO, CONH, NH, etc; n = 0 or 1), II (R1 and R2 = amidino or imidazolino; Z = CH:CH, NHN:N, etc.), III (X = O, S, or NH; Y = CH, CMe, N; R1 and R2 = amidino or imidazolino), and IV (X = NH; Y)= CH; Z = CH:CH; R1 and R2 = imidazolino; n = 0 or 1), were tested for antitumor activity against murine leukemia L1210 cells. Structure-function anal. revealed that the antitumor activity of the diarylamidines depended on the planarity of the mol., the presence of amidino or, preferably, imidazolino groups or both aryl moieties, the nature of the bridge connecting the 2 aryl moieties, and the nature of the aryl moieties (preferably benzofuren or benzo[b]thiophene. Thus, (6-(2-imidazolin-2-yl)-2-[4-(2-imidazolin-2-yl)phenyl]benzo[b]thiophene (I; X = S; Y = CH; R1 = R2 = imidazolino; n = 0) [73819-21-3] was the most potent inhibitor of L1210 cell growth. The inhibitory effects of diarylamidines on L1210 cell proliferation may at least partly involve an

inhibition of DNA synthesis. 2,2'-Vinylenedi-1-benzofuran-5-carboxamidine (III; X = 0; Y = CH; Z = CH:CH; R1 = R2 = amidino) [65426-90-6] exhibited potent antitumor activity in vitro and in vivo in L1210-inoculated mice.

IT 87559-26-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(neoplasm inhibitory activity of, structure in relation to)

RN 87559-26-0 HCAPLUS

CN 1H-Indole, 5-(4,5-dihydro-1H-imidazol-2-yl)-2-[4-[4-(4,5-dihydro-1H-imidazol-2-yl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

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FILE 'REGISTRY' ENTERED AT 13:43:42 ON 17 MAY 2004

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 26 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:06:23 ON 17 MAY 2004

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L5 0 S L3 AND PRIESTLEY, E?/AU

L6 0 S L3 AND DECICCO, C?/AU

L7 0 S L3 AND HUDYMA, T?/AU

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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